

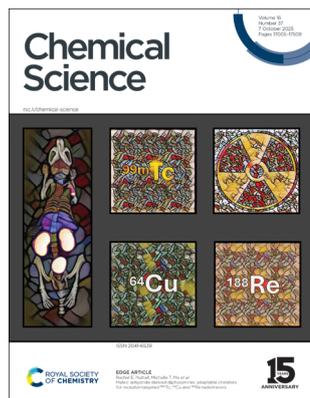
# Chemical Science

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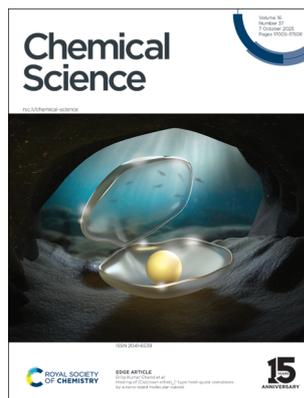
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## IN THIS ISSUE

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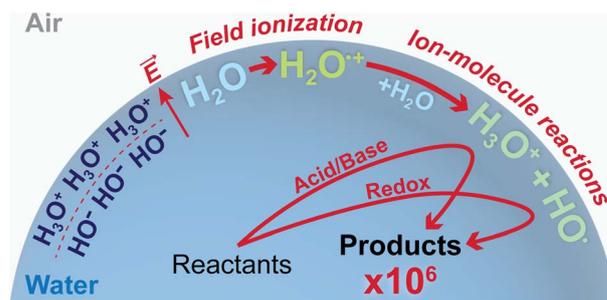
**Inside cover**  
See Dillip Kumar Chand *et al.*, pp. 17127–17138. Image reproduced by permission of Dillip Kumar Chand from *Chem. Sci.*, 2025, **16**, 17127.

## PERSPECTIVES

17020

### Mechanisms of ionization and of chemical reactions in charged microdroplets

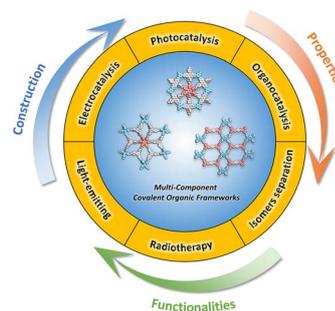
Dylan T. Holden, Brison A. Shira, Myles Quinn Edwards, Nicolás M. Morato and R. Graham Cooks\*



17034

### Multicomponent covalent organic frameworks: design strategies and synergistic functions

Xiaoyi Xu and Ning Huang\*



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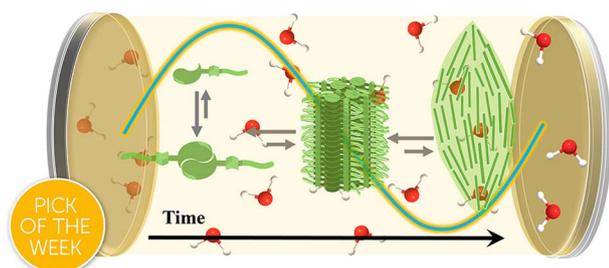
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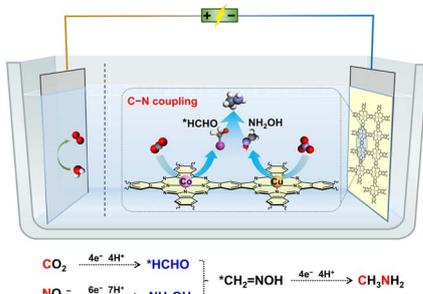
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### Impact of vibrational strong coupling on liquid-liquid phase separation in supramolecular polymers

Kripa Joseph, Hailin Fu, Joost J. B. van der Tol, Werner Steffen, Feixia Ruan, George Fytas\* and E. W. Meijer\*

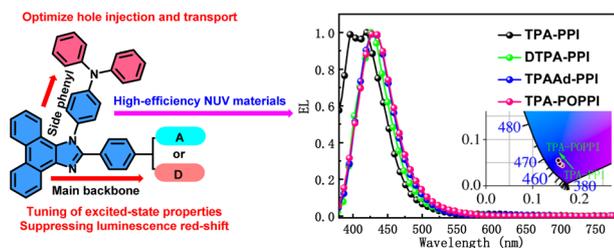
17148



### Electrocatalytic synthesis of methylamine from nitrate and carbon dioxide on a heterometallic polyphthalocyanine

Yiyang Zhou, Ruizhi Duan, Linqi Liu, Chunmei Ding\* and Can Li\*

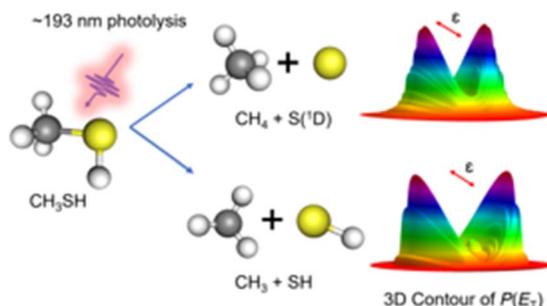
17156



### High-efficiency non-doped near-ultraviolet OLEDs achieved by regulating excited-state spatial distribution through molecular optimization to realize hybridized local and charge-transfer (HLCT) characteristics

Daokun Zhong, Ruiqin Zhu, Jie Zhang, Peng Tao, Bochao Su, Xiaolong Yang, Yuanhui Sun, Ling Yue, Guijiang Zhou\* and Wai-yeung Wong\*

17165



### Ultraviolet photodissociation of methanethiol ( $\text{CH}_3\text{SH}$ ): revealing an $\text{S}(^1\text{D})$ atom elimination channel

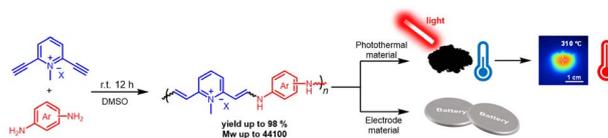
Yucheng Wu, Shunyang Zhou, Zijie Luo, Shuaikang Yang, Zhenxing Li, Yongxin Dong, Wei Hua, Quan Shuai, Dongxu Dai, Michael N. R. Ashfold,\* Kaijun Yuan\* and Xueming Yang



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### Spontaneous amino–yne click polymerization enabled by pyridinium-activated alkynes toward p– $\pi$ conjugated ionic polymers

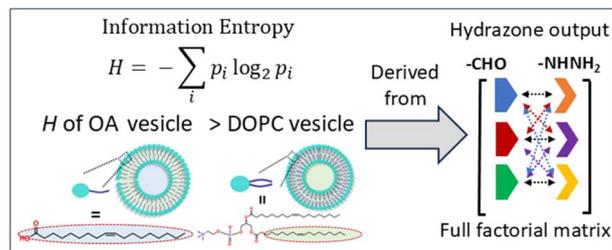
Chunyang Li, Guoqun Zhang, He Xu, Linjing Wei, Wuhua Liu, Kaiwei Zhang, Bingnan Wang, Chengliang Wang,\* Anjun Qin\* and Ben Zhong Tang



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### Decoding information entropy of fatty acid and phospholipid vesicles via ordering combinatorial output of hydrazones

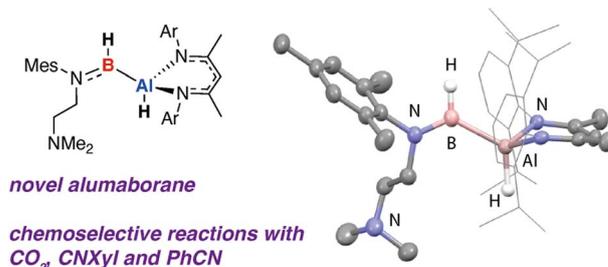
Reena Yadav, Niranjani Adikessavane, Rishi Ram Mahato and Subhabrata Maiti\*



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### Synthesis, properties, and chemoselective reactions of an AlH–BH functional group

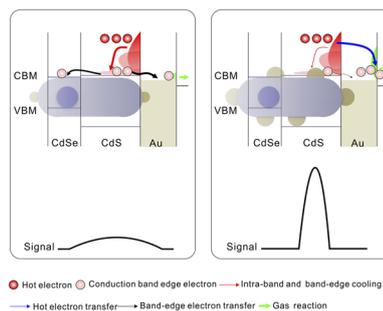
Wenbang Yang, Andrew J. P. White and Mark R. Crimmin\*



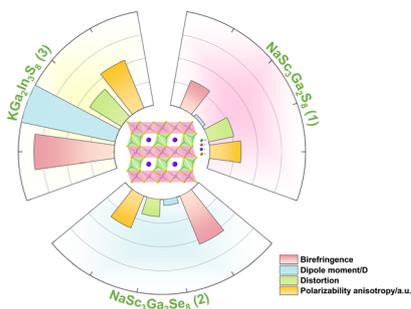
17200

### Harnessing non-equilibrium hot electrons in a quantum-engineered ternary heterostructure for sub-ppb C9 biomarker detection

Xiao Li, Wenyuan Zhao, Jiaying Liu, Rong Li, Sitong Jia, Cancan Li, Deyu Bao, Shan Zhu,\* Peng Wang, Lei Huang, Songqiu Yang,\* Miao Yu, Xiang Liu, Zhenjie Xue and Tie Wang\*



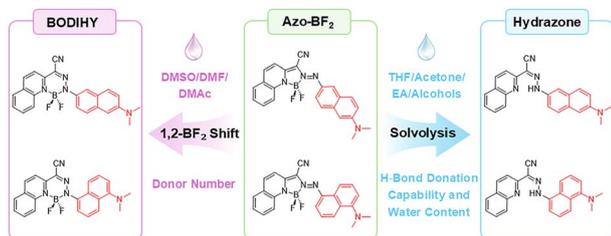
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### From $\text{NaSc}_3\text{Ga}_2\text{Q}_8$ ( $\text{Q} = \text{S}, \text{Se}$ ) to $\text{KGa}_2\text{In}_3\text{S}_8$ : substitution of $\text{Sc}^{3+}$ with $\text{In}^{3+}$ to achieve doubled birefringence

Yun Xie, Wen-Dong Yao,\* Qiu-Yang Du, Wenfeng Zhou, Nian-Tzu Suen, Wenlong Liu and Sheng-Ping Guo\*

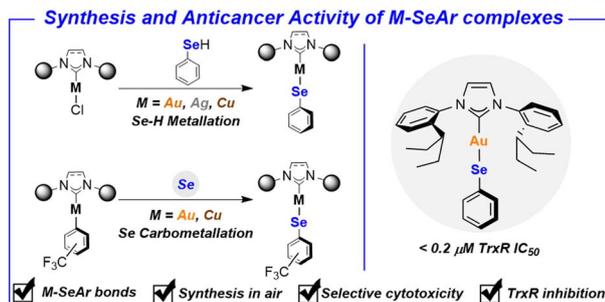
17214



### Solvent-dependent reactivity of azo- $\text{BF}_2$ switches

Qingkai Qi, Heyifei Fu, Lingya Peng, Shefali Patra, Xiaogang Liu and Ivan Arahamian\*

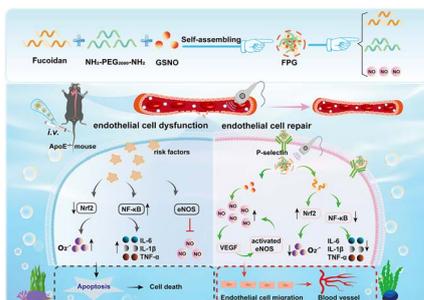
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### A new generation of N-heterocyclic carbene (NHC) gold-selenolato complexes as potent anticancer agents: distinct synthetic routes and evaluation in 2D and 3D cancer models

Pierre Arnaut, Nestor Bracho Pozsoni, Denys Bondar, Petra Lippmann, Susanne Boschuk, Ivan Semenyuta, Subhrajyoti Bhandary, Kristof Van Hecke, Yevgen Karpichev, Enrico Cavarzerani, Vincenzo Canzonieri, Flavio Rizzolio, Thomas Scattolin, Georgios C. Vougioukalakis, Ingo Ott,\* Nikolaos V. Tzouras\* and Steven P. Nolan\*

17232



### A natural ultrasound-triggered nitric oxide booster for endothelial dysfunction therapy

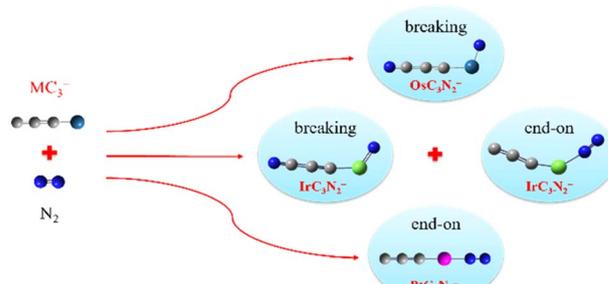
Yuqiong Wang, Dong Meng, Yu Dong, Xiaoqing Huang, Liping Wang,\* Wen Gao\* and Bo Tang



17241

### Observation of competing nitrogen activation in metal tricarbonyl anions $MC_3^-$ ( $M = Os, Ir, Pt$ )

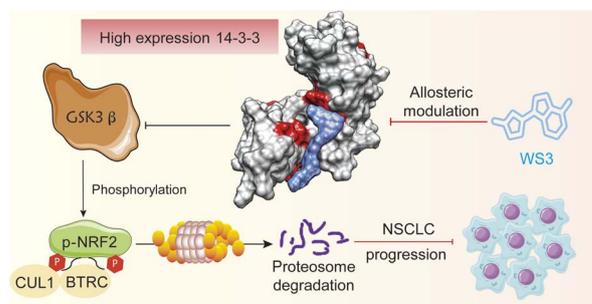
Shihu Du, Ziheng Zhang, Gang Li, Shibo Cheng, Xiangtao Kong, Lu Li, Qinqin Yuan, Hua Xie\* and Ling Jiang



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### Discovery of an allosteric 14-3-3 inhibitor for suppressing NRF2-driven cancer *via* phenotypic screening and chemoproteomic-based target deconvolution

Jinglong Zhao, Han Jiang, Kaimei Zhao, Tian Liu, Qiong Zhang, Ziquan Zhao, Junjie Wang, Qidong You,\* Mengchen Lu\* and Zhengyu Jiang\*



17261

### Metal-free pyridinium salts with strong room-temperature phosphorescence and microsecond radiative lifetime

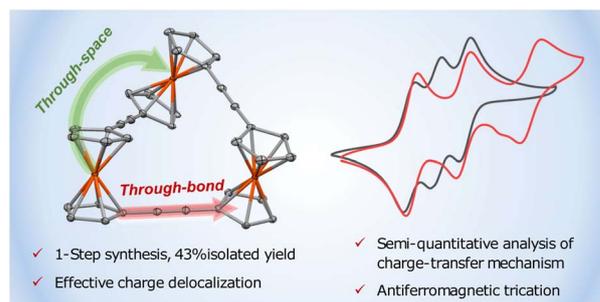
Eetu Hakkarainen, Hao-Cheng Lin, Anton A. Nechaev,\* Vsevolod A. Peshkov, Toni Eskelinen, Kai-Hsin Chang, Tzu-Hao Liao, Po-Yu Chen, Igor O. Koshevoy, Hao-Wu Lin,\* Pi-Tai Chou\* and Andrey Belyaev\*



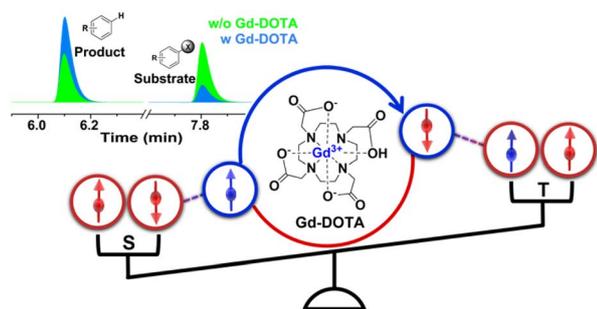
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### An acetylene-bridged ferrocene macrocycle: efficient synthesis and electron transfer mechanism in mixed-valence systems

Longfei Li, Beijing Zhang, Yi Xie, Qi Xiong, Yuanbo Zhong, Yansong Jiang, Yu Wang, Haobing Wang, Shang-Da Jiang, Shen Zhou\* and Xing Jiang\*



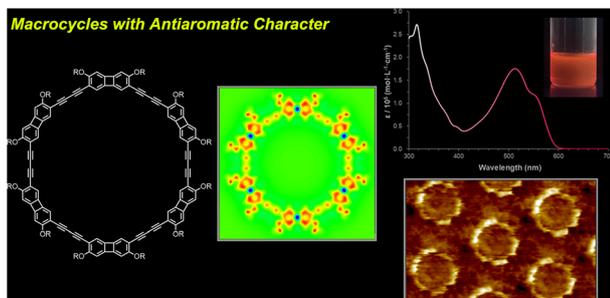
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### Enhancing photoredox catalysis by suppressing back electron transfer with the aid of a spin catalyst

Zhiqiang Dong, Chenli Chen, Lingfang Chen, Mingli Sun, Junzheng Zhan, Shen Zhou, Lijia Cao, Jianyu Liu, Shuming Bai,\* Jialong Jie,\* Hongmei Su, Song Gao and Linan Zhou\*

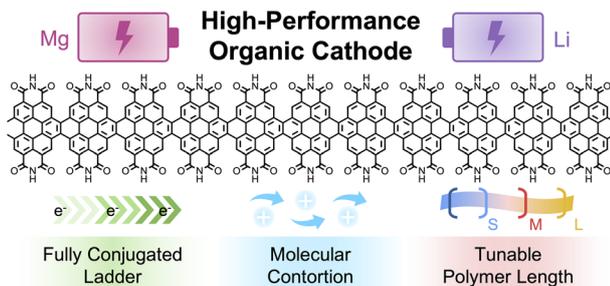
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### Macrocycles composed of biphenylene and butadiyne units with antiaromatic character

Shoko Nagayama, Hiroki Kawakatsu, Daisuke Asai, Takumi Yokoyama, Masahiro Yamashina, Shinji Toyota and Kazukuni Tahara\*

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### The "sweet spot" in length for contorted conjugated ladders in ultrafast-charging Li and Mg batteries

Wenrui Lei, Kelsey Harrison, Si Tong Bao, Kyunam Lee, Michael L. Steigerwald, Qian Cheng,\* Nicholas M. Orchanian,\* Colin Nuckolls\* and Qifeng Jiang\*

17304



### Molecular design of sensitizers for high-efficiency OLEDs: exploration of energy transfer dynamics

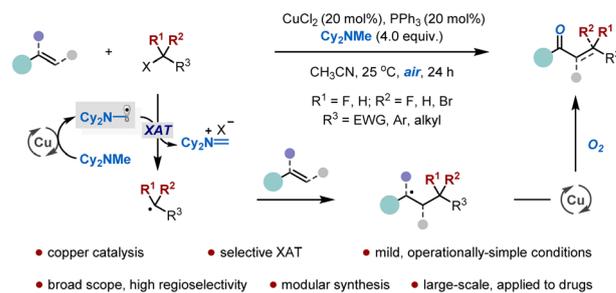
Xiao Liu, Xue-liang Wen, Yang Zhou, Chao Tang, Diandong Tang, Qian Wang, Yibo Shi, Lin Liu, Wei Sun, Kai Feng, Wei-Hai Fang,\* Juan Qiao,\* Lin Shen\* and Xuebo Chen\*



17316

### Copper-catalysed oxy-alkylation of styrenes enabled by halogen-atom transfer

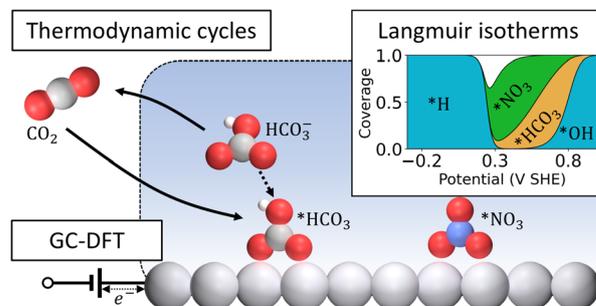
Qiujuan Tan, Xiang Lyu, Yu Zhao, Huaquan Fang,\*  
Xianxiu Xu\* and Zhongyan Hu\*



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### Predicting competitive anion electroadsorption on late transition metals

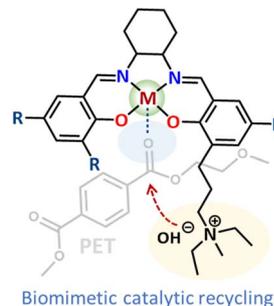
Bolton Tran\* and Bryan R. Goldsmith



17334

### Theory-guided multifunctional Zn-Salen molecular catalyst for sustainable polyester plastic recycling

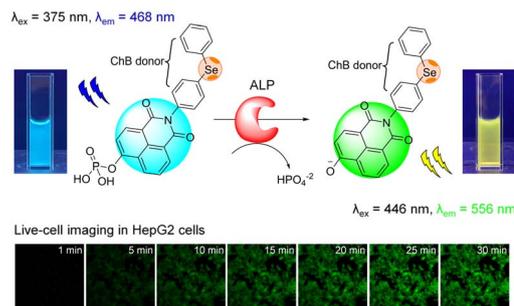
Mei Li, Yawen Shi, Lei Tang,\* Na Ji\* and Shengbo Zhang\*



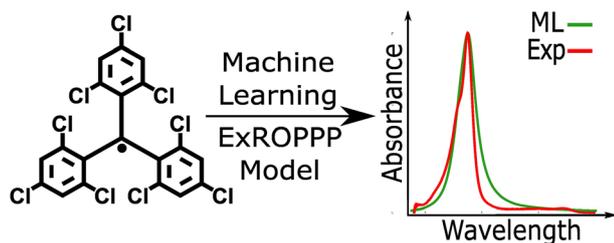
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### Tuning probe permeability via chalcogen and halogen atom substitution for monitoring alkaline phosphatase activity in mammalian cells

Ekta Chauhan, Debasish Giri, Harinarayana Ungati  
and Govindasamy Mugesh\*



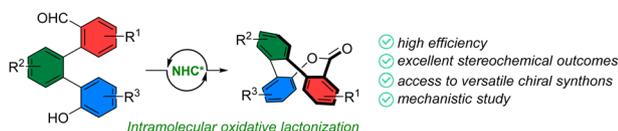
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### Learning radical excited states from sparse data

Jingkun Shen, Lucy E. Walker, Kevin Ma, James D. Green, Hugo Bronstein, Keith T. Butler and Timothy J. H. Hele\*

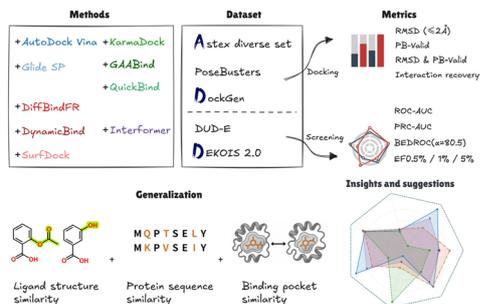
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### Enantioselective lactonization catalyzed by chiral N-heterocyclic carbenes enables access to inherently chiral eight-membered lactones

Vojtěch Dočekal,\* Adam Kurčina, Ivana Císařová and Jan Veselý\*

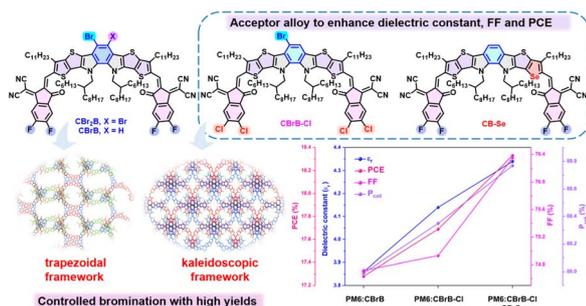
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### Decoding the limits of deep learning in molecular docking for drug discovery

Yue Li, Jiakai Yi, Hui Li, Kun Li, Fenghua Kang, Youchao Deng, Chengkun Wu, Xiangzheng Fu, Dejun Jiang\* and Dongsheng Cao\*

17391



### Effect of halogen/chalcogen substitution on the dielectric constant of asymmetric acceptor alloy to improve the efficiency and stability of inverted organic photovoltaics

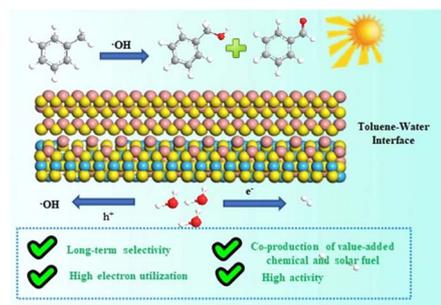
Yan-Bo Wang, Yung-Jing Xue, Chieh-Ming Hung, Kuo-Hsiu Huang, Bing-Huang Jiang, Chia-Lin Tsai, Yu-Chi Huang, Hong-Yi Chen, Shang-Da Yang, Su-Ying Chien, Chih-Ping Chen, Pi-Tai Chou\* and Yen-Ju Cheng\*



17408

### Dynamic surface radical confinement in a compact CdS–CdIn<sub>2</sub>S<sub>4</sub> semi-coherent heterojunction for highly efficient synergetic photocatalytic selective oxidation of toluene and enhanced hydrogen production

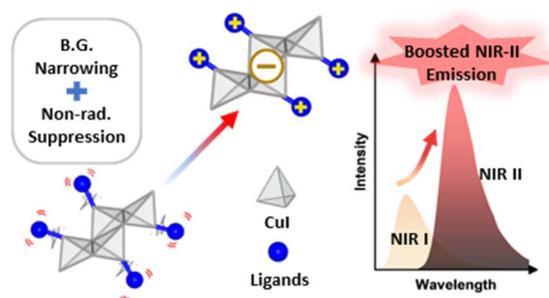
Yuhui Liu, Xiaoxu Deng,\* Chuangyun Guo, Shuang-Feng Yin\* and Peng Chen\*



17417

### Rigid cationic ligands enable high-efficiency NIR-II photoluminescence in copper(I) iodide hybrid semiconductors

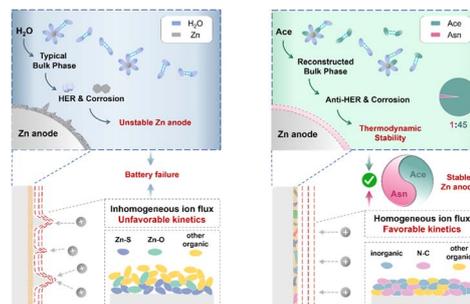
Jingwen Chen, Xueqian Wu, Minghui Zhang, Simon J. Teat, Guozhong Xu,\* Jingbai Li,\* Xiuze Hei\* and Jing Li\*



17426

### Concentration-function coupled electrolytes harmonize thermodynamics and kinetics for stable zinc metal batteries

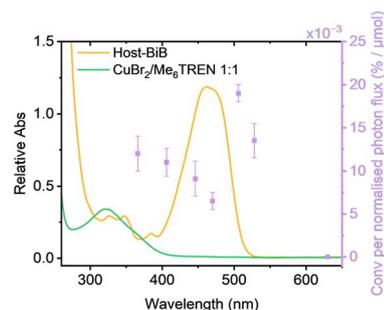
Tao Liu, Xusheng Dong, Jiashuo Zhang, Huihui Chen, Rongrong Cao, Zixu Sun, Wanhai Zhou, Hongpeng Li, Dongliang Chao, Zhen Zhou\* and Ruizheng Zhao\*



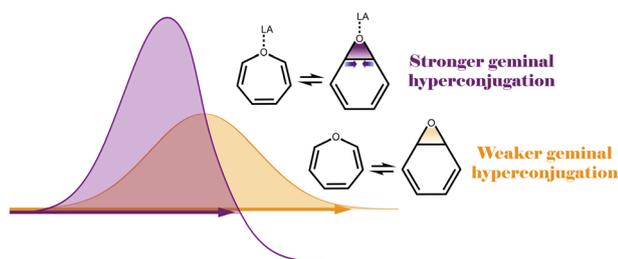
17436

### Visible-light-induced copper-mediated reversible deactivation radical polymerisation without additional photocatalysts

Mia D. Hall, Boyu Zhao, Evelina Liarou, Tanja Junkers\* and David Haddleton\*



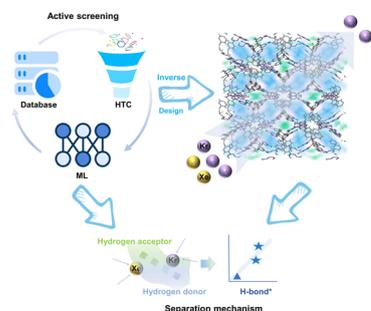
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### Geminal hyperconjugation as a driving force for C–C bond shortening in heavy-atom tunnelling

Croix J. Laconsay, Ishika Jain, Tim Schleif,\* William L. Karney\* and Judy I. Wu\*

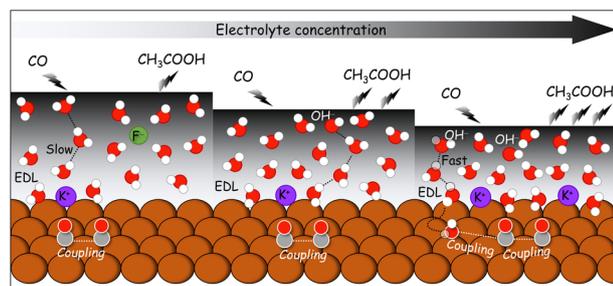
17450



### A mechanism-guided inverse engineering framework to unlock design principles of H-bonded organic frameworks for gas separation

Yong Qiu, Lei Wang, Letian Chen, Yun Tian,\* Zhen Zhou\* and Jianzhong Wu

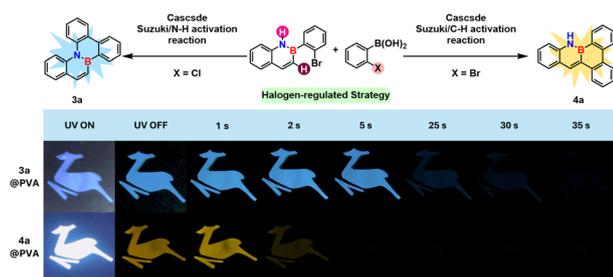
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### Atomic insights into how electrolyte concentration controls CO electroreduction to acetate

Xiaowan Bai, Lin Jiang and Yan Jiao\*

17470



### Regioselective construction of two isomeric BN-fused aromatic frameworks enabling the synthesis of ultralong room-temperature phosphorescence materials

Qiang Feng, Junxiong Yao, Qianxin Wu, Yang Qiu, Zicheng Wang, Xia Wang, Weilin Chen, Sibotong, Xiaohua Cao, Jianqi Sun, Qianqian Ye, Jianhua Liu,\* Dianyuan Wang,\* Jianguo Wang\* and Huanan Huang\*

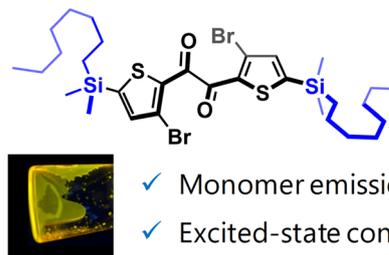


17480

### Fast and efficient room-temperature phosphorescence from metal-free organic molecular liquids

Yosuke Tani,\* Yuya Oshima, Rika Okada, Jun Fujimura, Yuji Miyazaki, Motohiro Nakano, Osamu Urakawa, Tadashi Inoue, Takumi Ehara, Kiyoshi Miyata, Ken Onda and Takuji Ogawa

### Solvent-Free Liquid RTP



$$\Phi_p = 5.6\% \text{ (air)}$$

$$25.6\% \text{ (Ar)}$$

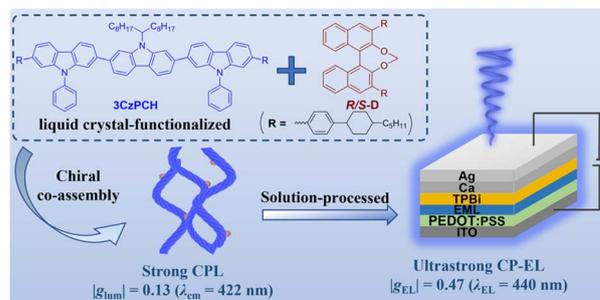
$$k_p = 6,900 \text{ s}^{-1}$$

- ✓ Monomer emission
- ✓ Excited-state conformation change

17487

### Ultrastrong circularly polarized electroluminescence achieved by chiral co-assembly of a liquid crystal-functionalized carbazole derivative

Hang Li, Dong Li, Zhenhao Jiang, Yuxiang Wang\* and Yixiang Cheng\*



17494

### The global kinetic–thermodynamic relationship derived from first principles

Eduardo Garcia-Padilla\* and Guanqi Qiu\*

full-range, **exact** kinetic-thermodynamic relationship fully deductive equation chemically **meaningful** parameters

